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13. ABSTRACT (Maximum 200 words)
The general objective of this research program is the development and application of new methods of analysis, numerical analysis, scientific computation visualization techniques within the context of specific nonlinear mechanics problems that model significant physical phenomena. In general mathematical terms the analysis and numerics can be classified as dealing with problems of continuation, bifurcation, and stability exchange as they arise in the variational principles of mechanics, and especially within the context of Hamiltonian systems. The fields of application all have these themes as common mathematical underpinnings, but specific models are as diverse as describing gravity-gradient effects on the attitude dynamics of large satellites, or the supercoiling and molecular dynamics of long-chain macro-molecules such as DNA. The guiding philosophy of the research is that substantial progress can be made by simultaneously considering context-specific modeling issues along with the development of new and generally applicable analytical and numerical techniques. Within the project there is a particular emphasis on the exploitation of computation combined with interactive visualization to provide understanding of data, and to generate insight and conjectures that lead to analytical conclusions.

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Briefer:

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\centerline{Applications of numerical continuation and visualization in
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The general objective of this research program is the development and
application of new methods of analysis, numerical analysis,
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within the context of specific nonlinear mechanics problems
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In the past year progress has been made in the following
areas:
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\noindent
{\bf A: Analysis}
Many systems can naturally be formulated as Lagrangian systems that are
subject to constraints. Consideration of
the dynamics of inextensible and unshearable rods (reference
[5] below) led to a novel {\it unconstrained} Hamiltonian formulation of a
rather

general class of such Lagrangian systems. The desired constraint is by
constructi on a
first integral of the Hamiltonian
dynamics. However the Hamiltonian, $H(x,y)$ say, is only defined after an
auxiliary minimization
$$
H(x,y)=\min_{\Lambda} \tilde H(x,y,\Lambda),
$$
where we call $\tilde H(x,y,\Lambda)$ the {\it pre-Hamiltonian}.
Here $y$ is the variable conjugate to the configuration variable $x$, but
in applications $y$ is typically not the classic momentum or impulse, and so
we give it a new name, the {\it impetus}. In applications the quantity
$\Lambda$ is generally the time anti-derivative of a familiar physical
quantity, e.g.\ for incompressible fluid flow (reference [6]) $\Lambda_t$ is the
pressure field. $\Lambda$ can also be interpreted as a Lagrange multiplier
enforcing a time-differentiated constraint, but to distinguish it from the
usual multiplier, we call $\Lambda$ the {\it striction}. In the context
of systems of ordinary differential equations the impetus-striction
formulation can be viewed as a variant of the vakonomic mechanics of Kozlov,
but the impetus-striction description naturally extends to systems of partial
differential equations. The new formulation has already proven effective in
obtaining analytical stability results [5], and numerical methods based
on the approach are currently under investigation.

The second analytical development concerns the effects of dissipation
on the characterization of stability properties in Hamiltonian systems
(Article [7] below).
The result is most simply stated in the case of equilibria of ordinary
differential equations. Consider the perturbed (autonomous,
canonical) Hamiltonian system
$$
\dot z = (J -\epsilon D) \nabla H(z),
$$
with $J$ skew and nonsingular, and $D$ symmetric and positive semi-definite.
Then the equilibria $z_e$ of the dynamics are precisely the critical points
of the Hamiltonian. For $\epsilon\ge 0$ it is easy to see
that minima of the Hamiltonian are necessarily
dynamically stable, and it is also known that in the case $\epsilon=0$
non-minima can also be dynamically stable (in the full nonlinear sense).
The new result states that for $\epsilon>0$ and for a natural class of
dissipations $D$ (including classic Rayleigh dissipation), the number of
unstable modes of the linearized dynamics coincides with the index of
$z_e$ regarded as a critical point of $H$. Special cases of this result trace
back to Kelvin, and are also of contemporary concern, but the generality
of this result, with no assumption on simplicity of eigenvalues for example,
is new. The result is significant because it allows effects of dissipation on
dynamic stability to be analyzed from a purely static, variational viewpoint.
The proof is a simple continuation argument that can also
be applied in the context of various Hamiltonian partial differential
equations.

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{\bf B: Applications areas}
Two areas of application have been of primary concern. The first concerns non-canonical Hamiltonian systems and gravity-gradient effects on the attitude dynamics of satellites. In an extension of completed but somewhat

qualitative work, and now in collaboration with Captain C.\ D.\ Hall of the Aerospace Engineering Department at the Air Force Institute of Technology (who is supervising a Ph.D.\ thesis on this topic) we are undertaking a quantitat ive investigation of whether the standard approximate model used for predicting steady-state attitudes of satellites can give incorrect answers in parameter regimes that arise for existing and envisioned satellite missions. The analytical and numerical projects concerning the dynamics of rods and effects of dissipative perturbations also pertain to this area of application because of issues arising with the motion of long aerials and tether systems.

The second area of application is the supercoiling of long chain molecules such as DNA. In the context of DNA the local atomic structure is known to be the classic double helix. The point of interest is how the double helix itself deforms and coils around itself or other objects such as proteins. This problem is of considerable contemporary interest to molecular biologists, chemists and mathematicians with a background in topology and knot theory (witness the IMA 1994 Summer Program in Topological Issues in DNA). However the heart of the probl em lies in issues of mechanics. Over the past year with a postdoc Y.\ Li we have developed a model for the equilibrium supercoiling of DNA both with and without e ffects of self-contact. From the outset the model has been developed to be amenable to efficient computation, but the formulation we use has also provided several analytical insights. By using modern theories of rod mechanics combined with the impetus-striction formulation mentioned above, the model is reduced to a two-point boundary value problem for a seven degree of freedom Hamiltonian system .
In the case of self-contact three of the ``ordinary" differential equations involve nonlocal terms expressed in terms of quadratures. In either case the problem can be efficiently discretized by the collocation method, and we have bee n using a solver and path following algorithms that are adaptations of the package AUTO.

In addition to applications in modelling DNA, the work applies equally well to ot her long chain molecules. For example tropomyosin is a large ``coiled-coiled" molecule comprised of two alpha helices interwound with each other, and the overa ll molecular structure is of considerable interest to biochemists. Similar systems arise in many other large molecules that are of interest to the Air Force. One application is that such coiled-coiled molecules have considerable potential for use as substrates to make materials that are optically highly nonlinear. Joint investigations with Dr.\ Ruth Pachter of the Laser Hardening Division at th e Wright Paterson Materials Science Laboratory are pursuing this line of investigat ion.
At a completely different scale the same code can be used to model highly twisted

and contorted wires that arise in cross-disciplinary applications such as intravenous surgical techniques using guidewires, or the construction of deployab le
space structures or aerials with complicated, possibly knotted, geometries.

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{\bf C: Numerical Algorithms}
In joint work with a postdoc J.-M.\ Xu we have constructed conservative algorithms for the numerical integration of (autonomous) Hamiltonian systems of ordinary differential equations. The algorithms have the property that they exactly (to machine precision) conserve the Hamiltoni an
(if autonomous) and also all other known integrals of the continuous system. The main idea is to enforce a compatability condition between the choice of time step and the discretization of the gradient operator, in order to construct a discrete chain rule. This discrete chain rule automatically implies conservation of the Hamiltonian, and conservation of the other invariants can be guaranteed by a rather natural and simple projection technique that only involves the solution of a (small) linear system. So far a simple second-order scheme has been implemented and tested on various classic Hamiltonian systems, such as the Kepler problem. The results are extremely competitive with both general purpose, and symplectic integrators. Higher order, stable, multi-step methods such as Gear's BDF schemes can also be modified to be made conservative, but the resulting schemes are quite expensiv e
in terms of function evaluations, and it is as yet unclear whether the increase i n
order results in a corresponding increase in efficiency.

The most obvious motivation to construct conservative schemes for Hamiltonian sys tems is
a natural desire to conserve physical quantities such as energy and angular momen tum.
However numerical implementations based upon the impetus-striction formulation of constrained Lagrangian systems as unconstrained Hamiltonian systems provides another compelling motivation. In such systems the constraints are by constructio n
integrals of the (continuous) Hamiltonian system, and so it is desirable that the y
be preserved by the numerical algorithm in order for the system to make sense.

%DAE's and molecular dynamics

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{\bf D: Scientific Computation and Visualization}
The group is involved in a number of projects exploiting advanced visualization techniques combined with interactive computation in parameter dependent problems.

Much of this work is done by calling customized computational code from within the commercial graphics package AVS. For development purposes practically all of the computation is
run on a small local cluster of DEC alpha workstations with Kubota graphics accel erators on two
machines. However some calculations are carried out remotely on the San Diego Cray, and on the University of Maryland CM5.
Working within the AVS package vastly decreases the required graphics programming

time, and allows effort to be concentrated on the scientific and numerical issues. One project is the continued development of the package MC^2 (Multiplie r
and Constraint Continuation) which allows interactive exploration of the set of critical points of two-parameter variational principles, with simultaneous display of various projections of the bifurcation surface, and determination of stability properties. The current version of MC^2 is particularly optimized to explore the sets of equilibria and relative equilibria of Hamiltonia n
systems of ordinary differential equations as arise, for example, in the steady-spins of satellites affected by external fields. In the past year, progress
has been made toward extension to analogous systems of partial differential equat ions
in time and one space dimension. Then the problem to be treated by MC^2 is a two-point boundary value problem for a nonlinear system of ordinary differential equations governing steady-state solutions. For such systems a very natural
data compression is immediately available. Once the two-point boundary value problem has been solved, by parameter
continuation methods combined with collocation or whatever other approach is desi red,
the only data that need be stored are an appropriate set of initial conditions fo r each
parameter value. All other data can be easily, and essentially instantaneously, r ecovered
by running an appropriate initial value-problem solver. The package PCR (develope d
by Domokos and Paffenroth) exploits this
idea to provide a graphics based tool for understanding bifurcation problems. Two graphics windows are provided, one displays four scalars along the (locally) one-dimensional families of solutions using three dimensional

coordinates plus a color scale.
Points on these curves can be selected by a single mouse-click, which causes the appropriate initial data to be sent to the initial value problem solver, and an appropriate projection of the actual solution for that parameter value is displayed in a second window. The tool is designed for general use, but has been developed and used extensively in the specific context of the DNA modelling problem described above. There the graphical display

of the solution allows the knot type, and contact regions to be easily understood, and the graphical connection between points in the bifurcation diagra m and the
corresponding solution lays bare the (quite complicated) symmetry relations betwe en
solutions on different branches.

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\centerline{\bf Articles Appeared, Accepted or Submitted in Last Year}
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\smallskip\itemitem{1.}(with J.C. Alexander)
``Bounds on the friction-dominated motion of a pushed object'',
Int. J. Robotics Research, {\bf 12} \#3 (1993) pp.~231--248
\smallskip\itemitem{2.}(with R.L. Sachs) ``On the stability of KdV multi-solitons '',
Comm. Pure and Applied Math. {\bf 46} (1993) pp.~867--901
\smallskip\itemitem{3.}(with D.J. Dichmann) ``Conservation laws in the

dynamics of rods", J. Elasticity, 1994, to appear
\smallskip\itemitem{4.}(with R. Nair) ``On the forward kinematics of
parallel manipulators", Int. J. Robotics Research,. {\bf 13} \#2 (1994)
pp.~171--188
\smallskip\itemitem{5.}(with D.J. Dichmann and R.L. Pego)
``Hamiltonian dynamics of an elastica and the stability of solitary waves",
Arch. Rat. Mech. Anal. (37 pages) to appear
\smallskip\itemitem{6.}(with R.L. Pego) ``An unconstrained Hamiltonian
formulation for incompressible fluid flow" (14 pages) Comm. Math. Physics,
submit ted
\smallskip\itemitem{7.}(with M.L. Overton)
``Stability Theory for Dissipatively Perturbed Hamiltonian Systems"
(26 pages) Comm. Pure Applied Math, submitted
\smallskip\itemitem{8.} (with R.L. Sachs) ``Constrained Variational Principles
an d Stability
in Hamiltonian Systems", to appear in ``{\it Hamiltonian Dynamical Systems}",
{\s 1 IMA
Volumes in Mathematics and Its Applications}, Eds. S.~Dumas , K.~Meyer and
D.~Schmidt.
(30 pages)
\smallskip\itemitem{9.} (by R.\ C.\ Paffenroth and G.\ Domokos) ``PCR-A
Visualiza tion
Tool for Multi-Point Boundary Value Problems" Institute for Physical Science and
Technology,
Technical Report, BN-1167, (1994)
\bye
On the analytical side there have been two significant developments.
The first constructs an unconstrained Hamiltonian formulation of the
dynamics of constrained Lagrangian systems. The second describes the effects
of dissipative perturbations on the stability analysis of special solutions,
such as equilibria and relative equilibria, in Hamiltonian dynamical systems.

Then a central issue is to describe the time
evolution of the Lagrange multiplier (or reactive `force') that maintains
the constraint. Perhaps the most familiar example is incompressible fluid
flow where the evolution of the pressure field is in question. In the
context of fluids the problem has been much analyzed, and there are many
schemes for resolving the difficulties, either by updating the pressure
field explicitly, or by taking representations such as vorticity where the
pressure drops out of the governing equations. However incompressiblity,
while certainly a very important case, is a comparatively simple constraint
from an analytical point of view.

his analysis is now moving into a more quantitative phase where the issue is
whet her
the size of these effects is of practical importance in the precise

This investigation is being pursued on two fronts. The first involves
collaborati on
with
Second, a proposal to the Industrial Mathematics Postdoctoral Program at the
National Science Foundation has been recommendend for funding by the Program
Offi cer,
and we are anticipating final approval at any time. That proposal is joint
betwee n the
University of Maryland and Computer Sciences Corporation, and would fund a
postdo c to
work on the satellite attitude dynamics problem using flight data from past and
p resent
NASA missions, and future mission designs.